Pair contact process with diffusion: A new type of nonequilibrium critical behavior?

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In the preceding article Carlon *et al.* investigate the critical behavior of the pair contact process with diffusion. Using density matrix renormalization group methods, they estimate the critical exponents, raising the possibility that the transition might belong to the same universality class as branching annihilating random walks with even numbers of offspring. This is surprising since the model does not have an explicit parity-conserving symmetry. In order to understand this contradiction, we estimate the critical exponents by Monte Carlo simulations. The results suggest that the transition might belong to a different universality class that has not been investigated before.

Symmetries and conservation laws are known to play an important role in the theory of nonequilibrium critical phenomena [1]. As in equilibrium statistical mechanics, most phase transitions far from equilibrium are characterized by certain universal properties. The number of possible universality classes, especially in $1+1$ dimensions, is believed to be finite. Typically each of these universality classes is associated with certain symmetry properties.

One of the most prominent universality classes of nonequilibrium phase transitions is directed percolation (DP) [2,3]. According to a conjecture by Janssen and Grassberger, any phase transition from a fluctuating phase into a *single* absorbing state in a homogeneous system with short-range interactions should belong to the DP universality class, provided that there are no special attributes such as quenched disorder, additional conservation laws, or unconventional symmetries [4,5]. Roughly speaking, the DP class covers all models following the reaction-diffusion scheme $A \leftrightarrow 2A$, $A \rightarrow \emptyset$. Regarding systems with a single absorbing state the DP conjecture is well established nowadays. However, various systems with infinitely many absorbing states have been found to belong to the DP class as well [6–8].

Exceptions from DP are usually observed if one of the conditions listed in the DP conjecture is violated. This happens, for instance, in models with additional symmetries. An important example is the so-called parity-conserving (PC) universality class, which is represented most prominently by branching annihilating random walks with two offspring $A \rightarrow 3A$, $2A \rightarrow \emptyset$ [9–11]. In $1+1$ dimensions this process can be interpreted as a Z_2-symmetric spreading process with branching-annihilating kinks between oppositely oriented absorbing domains. Examples include certain kinetic Ising models [12], interacting monomer-dimer models [13], as well as generalized versions of the Domany-Kinzel model and the contact process with two symmetric absorbing states [14].

A very interesting model, which is studied in the present work, is the $(1+1)$-dimensional pair contact process (PCP) $2A \rightarrow 3A$, $2A \rightarrow \emptyset$ [15]. Depending on the rate for offspring production, this model displays a nonequilibrium transition from an active into an inactive phase. Without diffusion the PCP has infinitely many absorbing states and the transition is found to belong to the universality class of DP. The pair

contact process with diffusion (PCPD), however, is characterized by a different type of critical behavior. In the inactive phase, for example, the order parameter no longer decays exponentially; instead it is governed by an annihilating random walk with an algebraic decay. Moreover, the PCPD has only two absorbing states, namely, the empty lattice and the state with a single diffusing particle. For these reasons the transition is expected to cross over to a different universality class. The PCPD, also called the annihilation/fission process, was first proposed by Howard and Täuber [16] as a model interpolating between ''real'' and ''imaginary'' noise. Based on a field-theoretic renormalization group study, they predicted non-DP critical behavior at the transition.

In the preceding article, Carlon, Henkel, and Schollwöck [17] investigate a lattice model of the PCPD with random-sequential updates. In contrast to Ref. [16], each site of the lattice can be occupied by at most one particle, leading to a well-defined particle density in the active phase. Performing a careful density matrix renormalization group (DMRG) study [18,19], Carlon *et al.* estimate two of four independent critical exponents. Depending on the diffusion rate d, their estimates for $\theta = z$ vary in the range $1.60(5)$–$1.87(3)$ while $\beta/\nu_\perp$ is found to be close to 0.5. Since these values are close to the PC exponents $z = 1.749(5)$ and $\beta/\nu_\perp = 0.499(2)$, they suggest that the transition might belong to the PC universality class.

The conjectured PC transition poses a puzzle. In all cases investigated so far, the PC class requires an *exact* symmetry on the level of microscopic rules. In $1+1$ dimensions this symmetry may be realized either as a parity conservation law or as an explicit Z_2 symmetry relating two absorbing states. In the PCPD, however, the dynamic rules are neither parity conserving nor invariant under an obvious symmetry transformation. Yet how can the critical properties of the transition change without introducing or breaking a symmetry? As a possible way out, there could be a hidden symmetry in the model, but we have good reasons to believe that there is no such hidden symmetry or conservation law in the PCPD. This would imply that the PC class is not characterized by a ''hard'' Z_2 symmetry on the microscopic level; rather, it may be sufficient to have a ''soft'' equivalence of two different absorbing states in the sense that they are reached by the dynamics with the same probability.
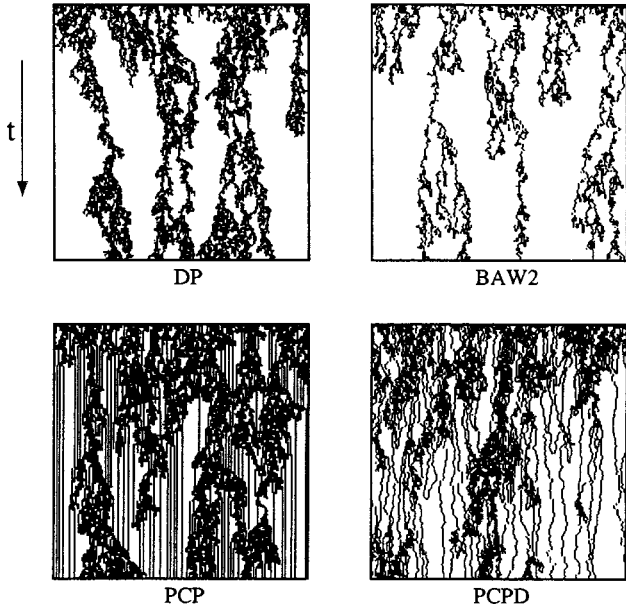
FIG. 1. Typical space-time trajectories of four different critical nonequilibrium processes starting with a fully occupied lattice. The four panels show directed percolation (DP), a branching-annihilating random walk with two offspring (BAW2), and the pair contact process without (PCP) and with (PCPD) diffusion.

In this paper I suggest that the transition in the PCPD might belong to a different, yet unknown, universality class. The reasoning is based on the conservative point of view that a ''soft'' equivalence between two absorbing states is not sufficient to obtain PC critical behavior. As described in Ref. [14], the essence of the PC class is a competition between two types of absorbing domain that are related by an *exact* Z_2 symmetry. Close to criticality these growing domains are separated by *localized* regions of activity. In $1+1$ dimensions, these active regions may be interpreted as kinks between oppositely oriented domains, which, by their very nature, perform an unbiased parity-conserving branching-annihilating random walk. In the PCPD, however, it is impossible to give an exact definition of ''absorbing domains.'' We can, of course, consider empty intervals without particles as absorbing domains. Yet, what is the meaning of a domain with only one diffusing particle? And even if such a definition were meaningful, what would be the boundary between an empty and a ''single-particle'' domain? Moreover, in PC models there are two separate sectors of the dynamics (namely, with even and odd particle numbers), whereas there are no such sectors in the PCPD. In fact, even when looking at typical space-time trajectories, the PCPD differs significantly from a standard branching-annihilating random walk with two offspring (see Fig. 1). In particular, offspring production in the PCPD occurs spontaneously in the bulk when two diffusing particles meet, whereas a branching-annihilating random walk generates offspring all along the particle trajectories. Therefore, it is reasonable to expect that the two critical phenomena are not fully equivalent.

In order to investigate this question in more detail, it is useful to compare the DMRG estimates with numerical re-
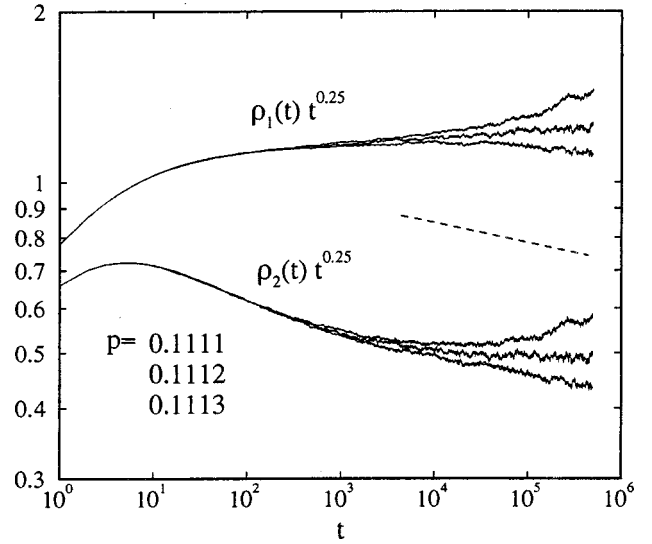

FIG. 2. The density of particles $\rho_1(t)$ and the density of pairs $\rho_2(t)$ times $t^{0.25}$ as a function of time measured in Monte Carlo steps. Upward (downward) curvature indicates deviations from the critical point. The dashed line represents the slope corresponding to the PC exponent $\delta \simeq 0.285$.

sults obtained by Monte Carlo simulations. It is important to note that there are two possible order parameters, namely, the particle density

$$\rho_1(t) = \frac{1}{L} \sum_i s_i(t) \qquad (1)$$

and the density of *pairs* of particles

$$\rho_2(t) = \frac{1}{L} \sum_i s_i(t) s_{i+1}(t), \qquad (2)$$

where L is the system size and $s_i(t) = 0,1$ denotes the state of site i at time t. Performing high-precision simulations it turns out that the critical behavior at the transition is characterized by unusually strong corrections to scaling [20]. These scaling corrections are demonstrated in Fig. 2, where the temporal decay of the two order parameters for $d = 0.1$ is shown as a function of time running up to almost 10^6 time steps. The pronounced curvature of the data in the double-logarithmic plot demonstrates the presence of strong corrections to scaling. Interestingly, the two curves bend in opposite directions and tend toward the same slope. Thus, in contrast to the mean-field prediction, $\rho_1(t)$ and $\rho_2(t)$ seem to scale with the same exponent. Discriminating between the negative curvature of $\rho_1(t)$ and the positive curvature of $\rho_2(t)$, we estimate the critical point and the exponent $\delta = \beta/\nu_\parallel$ as

$$p_c = 0.1112(1), \quad \delta = \beta/\nu_\parallel = 0.25(2). \qquad (3)$$

While this estimate deviates only slightly from the known PC value 0.286(2), other exponents deviate more significantly. Performing dynamic simulations starting with a single pair of particles [21], we measure the survival probability $P(t)$ that the system has not yet reached one of the

two absorbing states [23], the average number of particles $N_1(t)$ and pairs $N_2(t)$, and the mean square spreading from the origin $R^2(t)$ averaged over the surviving runs. At criticality, these quantities should obey asymptotic power laws, $P(t) \sim t^{-\delta'}$, $N_1(t) \sim N_2(t) \sim t^{\eta}$, and $R^2(t) \sim t^{2/z}$, with certain dynamical exponents δ' and η. Notice that in non-DP spreading processes the two exponents $\delta = \beta/\nu_{\parallel}$ and $\delta' = \beta'/\nu_{\parallel}$ may be different. Going up to 2×10^5 time steps we obtain the estimates

$$\delta' = 0.13(2), \quad \eta = 0.13(3), \quad z = 1.83(5). \quad (4)$$

Although the precision of these simulations is only moderate, the estimates differ significantly from the PC exponents $\delta' = 0.286$, $\eta = 0$ in the even sector and $\delta' = 0$, $\eta = 0.285$ in the odd sector. The exponent z, on the other hand, seems to be close to the PC value 1.75.

The most striking deviation is observed in the exponent β, which is not accessible in DMRG studies. Here the estimates seem to decrease with increasing numerical effort. As an upper bound we find

$$\beta < 0.67. \quad (5)$$

Even more recently, Ódor studied a slightly different version of the PCPD on a parallel computer, reporting the estimate $\beta = 0.58(1)$ [22], which is incompatible with the PC exponent $\beta = 0.92(2)$.

In summary, the critical behavior of the PCPD is affected by strong corrections to scaling, so that it is extremely difficult to estimate the critical exponents. Although DMRG estimates presented in [17] are very accurate, they have to be taken with care since they are affected by scaling corrections as well. Thus, the apparent coincidence with the exponents of the PC class may be accidental. Comparing other exponents, in particular the density exponent β and the cluster exponents δ' and η, the PC hypothesis can be ruled out.

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